File: anaflex-3b.pdf

ANAFLEX

Version 3b, January 2014

INDEX

1. Introduction and main input file
2. Mode 1: Steady state properties
3. Mode 2: Time-dependent properties
4. Mode 3: Correlation functions
5. Mode 4: Visualization
6. Mode 9: Trajectory
7. Output files
8. Release notes

1. Introduction and main input file

This program is intended for the analysis of the Brownian dynamics trajectories generated by **`BROWFLEX`**. It can work in one of the following five ways (working modes):

(1) Steady-state calculation. This is intended for steady-state values of the observable properties, which will be obtained as averages over the whole trajectory of the instantaneous values of the properties of a single molecule.
(2) Time-dependent calculation. This is intended for tracking the time evolution of properties of a sample of molecules. At each time, the sample average will be determined, thus obtaining the time-evolution of the properties of the sample.
(3) Correlation function calculation. This is intended to compute some usual time correlation functions and obtaine some relaxation times.
(4) Record coordinates for graphics display ("picture" or "movie").
(5) Convert the output binary trajectory file into a text file.

The program can process any number of cases in the same run. The input data files are the main data file (**`datafile`**) and one or several trajectory files (**`trajfile1`**, **`trajfile2`**…). When program **`ANAFLEX`** is launched it asks for the name of the main input file that contains all the information required as described below.

Main input data file

The **`datafile`** contains the following lines:

(a) FIRST PART (general for all of the working modes)

- **`logfile`**, is the name of the output file containing error messages, intermediate results and also some final results
- **`resfile`**, is the name of the output file containing final results

- **sumfile**, is the name of a tabular summary results file, ready to be exported to spreadsheets or other programs
- **nfrec**, is the sampling frequency of the records in the trajectory file. For instance, if this value is 10, one out of 10 consecutive records in the trajectory file will be used for the statistical (averages) calculation
- **instprofiles**, if =1 then files with instantaneous values along time of each property will be written in the working directory. These files will be named after the Fortran unit, which will be 31, 32, 33,... For example, in Compaq/Digital Fortran they appear as fort.31, fort.32,... The succesive files are for the succesive trajectories analized in the same run of **ANAFLEX**.
- **mode**, indicates the working mode of the program. The five possible values are **mode** =1 steady-state properties; **mode** =2 time-dependent properties; **mode** =3 correlation function; **mode** =4 for graphical display; **mode** =9 for converting the binary trajectory file into a text file.

(b) SECOND PART, depending on the mode. The lines in this block will be described in the following sections (sections 2, 3, 4, 5, 6).

(c) THIRD (FINAL) PART (again, general for all of the working modes)

- **trajfile1**, name of first trajectory file (not free format; fill with spaces up to 30 characters)
- .... successive lines with other trajectory files, if we are processing more than one
- * (asterisk) in place of **trajfile** indicates end-of-file

We recall that the trajectory file generated by an execution of **BROWFLEX** will contain a number **nmol** of subtrajectories in which the trajectory of a molecule has been subdivided, or a number **nmol** of molecules for different user-provided initial conformations.

2. Mode 1: Steady-state properties

This mode is intended for systems in steady state. Averages of the properties are evaluated for each subtrajectory. If **nmol** is not 1, estimates of the errors will also be given.

In this mode, the particular lines to be inserted in the main input file (i.e. block (b) SECOND PART above) are

- **ncodes**, **nprops**, two comma separated values which are

- **ncodes** is the number of groups of properties (or codes) to be computed (see below)
- **nprops** is total number of properties to be computed, i.e. total number of properties included in all of the groups considered in this run

Then there will be a number **ncodes** of lines. A line for each code (group), with

- **icode**, **ii**, **jj**, **kk**, **ll**, i.e. five comma separated values where

- **icode** is the code number of each group (see table below)

- **ii**, **jj**, **kk**, **ll** are four integer numbers (flags) which are needed for some groups of properties. If some or all of these values are not needed, then fill them with zeros.

Make sure that the total number of properties (sum over all of the groups) is exactly the value given as **nprops**.

As it has been already mentioned, the properties are grouped, each group containing one or more than one property. Each group has a code number. The following table lists the groups and their properties.

Code for group	**Number of properties**	**Properties**	**Description**
1	1	r^2_{1N}	1-N (linear end-to-end) square distance
2	1	s^2	Square radius of gyration
3	1	G_{zz}	Component of the gyration tensor
4	2	G_{xx} ,G_{yy}	Component of the gyration tensor
5	3	G_{xy} ,G_{xz},G_{yz}	Component of the gyration tensor
7	2	e_z, e_z^2	Extension along z, and its square
8	4	e_x, e_x^2, e_y, e_y^2	Extension along x and y,and their squares
12	1	Δn^*	Birefringence FENE chain (soft springs)
13	1	$<P_2>= \Delta n^*$	P_2 average over connectors (hard springs)
14	6	$\tau_{xx},\tau_{xy},\tau_{xz},\tau_{yy},\tau_{yz},\tau_{zz}$	Components of the stress tensor
18	6	$D_t,[\eta],D_r^{(1)},D_r^{(2)},D_r^{(3)},R_g$	Rigid-body hydrodynamic properties. Flag ii(=10, 11, 12) is the type of volume correction (see observations below)
20	5	R_ij^2, ^1, ^3, ^4, ^-1	Powers of distance Rij between beads I and J (given by unsing flags ii and jj)
24	5	Psi, psi^2, sin, cos, cos^2	Dihedral (torsion) angle (rad) subtended by beads I-J-K-L (given by using flags ii,jj,kk,ll). Zero is trans conformation.

Observations:

(a) The main direction of the external agent (flow, field) is z.

(b) Group 13, property $<P_2>$, is the birefringence Δn for a model of identical (quasi)rigid bonds.

Group 18, properties D_t, $[\eta]$, $D_r^{(1)}$, $D_r^{(2)}$, $D_r^{(3)}$ and Rg, are the translational diffusion coefficient, intrinsic viscosity, eigenvalues of rotational diffusion, and mean square radius of gyration, evaluated according to the rigid-body treatment, in which hydrodynamic properties of individual conformations are evaluated from a Kirwood-Riseman calculation with hydrodynamic interaction, like in the HYDRO++ program (please see the HYDRO++ User manual). Of the various options in HYDRO++ to treat the so-called volume correction, the one denoted as ICASE=12 (full volume correction

for $D_r^{(1)}$, $D_r^{(2)}$, $D_r^{(3)}$ and adjusted volume correction for [η]) is used. Please see the HYDRO++ User manual for further reference. This calculation takes a long computer time, and therefore a large value of **nfrec** (giving a small number of conformations for calculations) is recommended.

3. Mode 2: Time-dependent (transient properties)

This mode is intended for the evaluation of properties dependig on time. The result output files will contain the values of average properties as a function of time. For that purpose, a sample of **nmol** independent molecules should have been simulated (or, in other words, the simulation should have been repeated for **nmol** initial conformations).

The block (b) (SECOND PART above) in the main input file is the same as in mode 1 since the same properties can be evaluated. The difference is that now you get the time evolution of every property computed at every time as a sample average over the **nmol** molecules.

4. Mode 3: Correlation functions

This mode is intended for the evaluation of several time correlation functions, C(t). For that purpose, a long enough simulation at equilibrium with only one molecule (**nmol**=1) should have been performed. Alternatively, if **nmol** is not one, then the starting point of each molecule should be the end of the previous one (see instructions for **BROWFLEX**), so that the whole simulation is like the simulation of a single molecule in **nmol** succesive subtrajectories.

The block (b) (SECOND PART above) in the main input file consists of just one line with the following comma separated values:

- **indcorr**,**ian**,**inbase**,**ntimc**,**tmax**,**iii**,**jjj**,**nvx**,**vx(1)**,…**vx(nvx)**

where:

- **indcorr** indicates the type of correlation funcion (see table below)
- **ian** is the type of fitting of correlation function (usually 3, except 1 for translation). Possible values are:
  0: none
  1: C(t) = Qt
  2: ln C(t) = $c_1+c_2t+c_3t^2$+... (up to fourth-degree).
  3: C(t)=$a_1\exp(-b_1t)+a_2\exp(-b_2t)$+... (up to 5 exponentials), optionally including a base line.
- **inbase** is the indicator of base line in some types of fitting
- **ntimc** is the number of values (points) of the correlation function. It should be like 11, 21, 51… For multiexponential fits, values larger than 21 are advised.
- **tmax** is the maximum time reached in the calculation of the correlation function
- **iii**, **jjj** are bead indices needed in some cases. If not needed give `0`, `0`
- **nvx** is the number of values of **vx**, needed in some cases. If not needed give `0`
- **vx(1)**,…**vx(nvx)** values of **vx** (if **nvx** is not zero, otherwise they are omitted)

The correlation functions corresponding to the various values of **indcorr** are as follows:

indcorr	**Correlation function**	**Observations**
1	Overall translational diffusion, Dt	
5	$<P_2(\cos\theta)>$ for a vector joining two beads	iii and jjj are the indices of the two beads
9	Depolarized dynamic light scattering	
10	Polarized dynamic light scattering	vq(1),.... are scattering vectors
14	<Rij·Rij> where Rij is the vector joining beads I and J	iii and jjj are beads I and J
15	First Rouse mode	
16	Second Rouse mode	

The only function that needs **vq** values is polarized DLS (**indcorr**=10).

5. Mode 4: Visualization

This mode is intended to visualize snapshots or movies of the trajectory generated by **BROWFLEX**, using our visualization programs **VisualBeads** and **MovieBeads**, or any other graphics program.

The block (b) (SECOND PART above) in the main input file has the following lines:

- **igraph**, is a flag indicating the visualization mode
- **graphname**, is a character string with five (neither more nor less than five) characters
- **colorsfile**, is the name (up to 30 characters) of a file with indices for colors of beads and connectors (see below for valid colors). You can ommit this file if you do not want special colors; then in this line put a "-" (minus sign) as the first and only character and the program will take a standard combination of colors. Also, this file should be ommited in certain igraph modes (see below).

The content of **colorsfile** is a number of lines with the following information:
- **N**, the number of beads in the first line
- The following **N** lines consists of two values each one: the bead index (1…**N**) and the color index for that bead
- **NBONDS**, the number of connectors
- The following **NBONDS** lines consists of two values each one: the connector index (1…**NBONDS**) and the color index for that connector

Note that **N** and **NBONDS** must coincide with the values that were used in the **moleculefile** during the simulation; otherwise an error message will be issued. The valid color indices when **igraph** is 6 or 7 are

1 – WHITE ; 2 – RED ; 3 – YELLOW ; 4 – NAVY BLUE
5 – GREEN ; 6 – PINK ; 7 – SKY BLUE

We note that **colorsfile** is the file with colors of beads and bonds in the format valid for **VisualBeads** and **MovieBeads**. It will be needed for the production of graphics files in the formats accepted by these programs. In the present version, these are the cases when **igraph** = 6 or **igraph** = 7.

Types of recording (igraph) modes

With a sampling frequency given by **nfrec** (see above), a conformation will be recorded from the trajectory file. Thus, the number of conformations per molecule that are recorded is the number of conformations per molecule in the trajectory, **nconf**, divided by **nfrec**: **nconf**/**nfrec**. Then, the total number of conformations recorded for graphics purposes, **nconfgraph**, will be that ratio multiplied by the number of molecules, **nmol**, plus 1 because the initail conformation is also taking into account:
nconfgraph = **nconf***nconf/**nfrec** +1.
In general, **nconfgraph** should be reasonably small, say 11, 51...101. Its maximum value is 999.

The possible values of igraph are:

- **igraph**=1 (pdb format) is only valid when all the beads have the same same size (if they are not, an error message will be issued). In this mode, a series of files named **xxxxxnnn.pdb** will be produced. **xxxxx** is the (five character) string given for **graphname**, and **nnn** will be a three-digit index: 001, 002, ... up to **nconfgraph**. If **nconfgraph** exceeds 999, there will be an error message. As mentioned above, you will typically ask for a moderate **nconfgraph** (if not you will get so many files that may fill your disk!). The files **xxxxxnnn.pdb** have a Protein Data Bank format, and can be visualized using **RasMol** or similar molecular graphics tools. With **RasMol**, you can make /Display/Spacefill to view only the beads (with the real size), and also you can make /Display/Ball & Stick to visualize the beads (with a reduced size) and, what is quite interesting, the connectors.

- **igraph**=6 (Static VRML format) is valid for beads of arbitrarily different sizes. In this mode, a series of files named **xxxxxnnn.vrml** will be produced. **xxxxx** is the (five character) string given for **graphname**, and **nnn** will be a three-digit index: 001, 002, ... up to **nconfgraph**. If **nconfgraph** exceeds 999, there will be an error message. As mentioned above, you will typically ask for a moderate **nconfgraph** (if not you will get so many files that may fill your disk!). The files **xxxxxnnn.vrml** contain the coordinates and radii of the spheres in a full VRML format. For each image, our program sets "intelligently" the camera, lights, etc. (Note that the viewpoint varies from one image to another).

- **igraph**=7 (Animated VRML format) is valid for beads of arbitrarily different sizes. This mode is intended for trajectories generated with **nmol**=1, or (only in

special cases) with other **nmol** but such that the trajectory of a molecule is a continuation of that of the preceeding one. In this mode, a single file named **xxxxx-ani.vrml** will be produced. **xxxxx** is the (five character) string given for **graphname**. It will contain a number of snapshots equal to the number of files in the other modes (determined by the number of conformations in the trajectory and the sampling frequency, **nfrec**). The number of snapshots should be reasonably high, but not too much (if it is too large the VRML viewer may fail).

Static and animated VRML formats are among those considered by our separate visualization programs **VisualBeads** and **MovieBeads**. Please see the User Guides for these programs.

- **igraph**=8 (MOVIE formats) is valid for beads of arbitrarily different sizes. This mode is intended for trajectories generated with **nmol**=1, or (only in special cases) with other **nmol** but such that the trajectory of a molecule is a continuation of that of the preceeding one. In this mode, a single file named **xxxxx-mov.txt** will be produced. **xxxxx** is the (five character) string given for **graphname**. This file contains a header with information on the beads and connectors, and a series of snapshots, each given by a block of lines, one for each bead with the bead coordinates. This format is intended to be handled offline with any other user-supplied animated graphics program.

6. Mode 9: Trajectory file

This mode is just intended to transform the binary trajectory file generated by **BROWFLEX** into a text file that can be handled for any other user-supplied program.

In this mode, what has to be inserted in the main input file (indicated as block (b) SECOND PART above) is a single line containing

- **trajectext**, the user-supplied name of the text-formatted trajectory file

The content of this file is described below.

7. Output files

Trajectory file in text format

In **mode** 9, i.e. when the user intends to use his/her own analysis program, the only output file will be the trajectory file in text format, named **trajectext**. The contents of this file will be:

- name of the **inputfile** (main input file used in the **BROWFLEX** simulation)
- **nmol**(I), number of molecules (or subtrajectories of a single molecule).
- **ttraj**(R), time of duration of the subtrajectory of each molecule.

- **nconf(I)**, number of conformations (per molecule or subtrajectory) registered in the trajectory file, including the initial one. Thus, it will be the number of conformations (per molecule or subtrajectory) that was specified as an input parameter for **BROWFLEX** plus 1.
- **N(I)**, number of beads/atoms.

Then, there will be **nmol** blocks of lines, each containing **nconf** sub-blocks of lines – one for each recorded conformation – with each sub-block containing **N** lines, each with the three values of the coordinates x, y and z of each bead/atom.

Note that the time interval between successive conformations is **ttraj/nconf**.

A user-supplied analysis program would open **trajectext** and read its information as indicated above. It is likely that other information used by **BROWFLEX** could be needed. As the name of the main input file used by **BROWFLEX**, **inputfile**, is provided, the user program would open **inputfile**, which contains the names of the other, specific files, where all the input data used by **BROWFLEX** are contained.

The output files listed below does not appear in **mode** 9.

Log output file

File **logfile** will contain a description of the input parameters read from every one of the trajectories analyzed in a run, the possible error messages, and both intermediate and some final results.

Results output file

File **resfile** will contain the final results, including all the cases (trajectories) analyzed in a run. If **mode**=3 (correlation functions), the file informs about the time-dependence of the correlation function, details of the correlation analysis (multiexponential fits) and final results (relaxation times).

Summary output file

File **sumfile** will contain a summary of the results. The contents will depend on mode:

If **mode**=1 (steady-state), there will be a series of lines, one for each trajectory, with the following comma separated values:

param-f1, param-e1, prop1, +-, error1, prop2, +-, error2, prop3, +-, error3,...

where

- param-f1 and param-e1 are the first flow parameter and the first electric-field parameter (in the cases when there were any of this kinds of external agents). If simulation was performed without files containing flow and electric parameters (see **BROWFLEX** manual), -9.0 appears as the value of param-f1 or param-e1.
- prop# is the # property value, and error# is its error.

If **mode**=2 (time-dependent properties), the file contains blocks of data, one for each trajectory. Each block contains a series of lines, with the following (non-comma separated) values:

line# time param-f1 param-e1 prop1 +- error1 prop2 +- error2 prop3 +- error3...

where param*, prop* and error* have the same meaning as in **mode** =1, and time is the value of time.

If **mode** =3, the file is empty.

The errors are estimated dividing the sample of **nmol** molecules in 5 subsamples, therefore **nmol** must be a multiple of 5.

File **sumfile** can be easily exported to **Excel** or other spreadsheets or graphics programs for further analysis or visualization of various aspects, such as the dependence of properties on time, external agents, etc.

Other files

In **mode** =1 or 2, if **instprofiles**=1, the program will produce files, one file for each analyzed trajectory, containing the instantaneous values of the properties for each individual molecule in the sample. They serve to monitor how each individual molecule has evolved during the simulation. These files are named fort.21, fort.22....etc. They have blocks of lines, one for each molecule. Each block has the following data:

line#, time, param-f1, param-e1, prop1, prop2, prop3, ...

These files are particularly useful for "single-molecule" studies, as they provide how the properties of a single molecule, or each molecule in a sample, evolve during the dynamics trajectory.

7. Release notes

- Version 3b is the third released version of **ANAFLEX**.
- In this version, optimized mathematic libraries (MKL) are used to perform some vector and matrix operations.